

The Equation of Atom Motion in an External Gravitational Field.

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Abstract

It is shown that the motion of a multielectron atom in an external gravitational field in a good approximation is described by system of the Mathisson—Papapetrou equations, if we put as a classical angular momentum of the atom the expectation value of the operator of the full angular momentum of the system, which includes spins of the nucleus and electrons, and orbital momentums of the electrons in the atom.

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1 Introduction

The interest to the problem of the atom motion in an external gravitational fields is caused by the following two reasons.

First, the question about the possibility of using the atoms as the detectors of the gravitational fields represents the significant interest for modern astrophysics [1–4]. Second, because the atom is an extended quantum system, with the inner structure (the motion of extended bodies in general relativity is widely discussed in the literature), the problem of atom motion has considerable theoretical interest too.

The analysis of this situation shows, that the influence of an external gravitational field on the atomic spectra can reach the experimentally measurable values only in extremely strong gravitational fields (with characteristic radii of curvature $\leq 10^{-3}$ cm) [5,6,8], or in the case of ultrarelativistic motion of atom as a whole [8,10]. Apparently, in both cases the motion of an atom cannot be considered *a priori* as a geodesic one. So the finding of the equations of the atom motion in an arbitrary curved space-time is the important problem. For the case of the one-electron atom this problem was solved in the paper [9]. Following this work we shall generalize received results for the case of multielectron atom.

For essential simplification of the subsequent calculations, we shall use two assumptions. First, because nucleus mass μ is much greater than electron mass m ($\mu \gg m$), the atom motion can be considered in a good approximation as a motion of a classical point particle with the law of motion

$$x^i = \xi^i(\tau) \tag{1}$$

where τ is the proper time: $d\tau^2 = -c^{-2}ds^2$. Moreover, the assumed identity of atom and nucleus masses permits the consideration of the atomic motion as a nucleus one. Second, we shall describe the motion of electrons in the atom by quantum mechanics. Moreover, because the relative motion of electrons in the atom is the essential non-relativistic ($v \ll c$), so in the special comoving reference frame the atom can be described in frameworks of non-relativistic (or quasi-relativistic) quantum mechanics [8]. Subsequently we shall assume that the atom is in a quasistationary quantum state.

Thus, one can obtain the equation for $\xi^i(\tau)$ from the following suggested model. The nucleus, in the classical mass-point approximation with intrinsic angular momentum (spin), is moving in an external gravitational field and interacting with the electromagnetic field of the electrons. The electrons, which for their part is moving in external gravitational field and in the electromagnetic field of the nonexcited and electrons, are considered in a quasistationary bound quantum state.

We notice, that this assumptions are usual. It allows us instead of the relativistic problem of many bodies, which even in flat space has a lot of difficulties¹, consider the motion of electrons in the given electromagnetic field, created by a nucleus, and also in an external gravitational field.

As it is shown in works [7, 8], the generalized Ehrenfest theorem was proved for a Dirac particle in quasi-classical approximation. According to this theorem,

¹Quantum mechanical problem of two bodies in a weak gravitational field was discussed in work [11].

the expectations values of the position and spin operators of a electron fulfill the Mathisson—Papapetrou equations [12,13], which are describing a motion of a classical particle with a spin in an external gravitational field. Applying this results (valid for any Dirac particles) to the nucleus is represented justified. Therefore, to describe the nuclear motion in our model, we will use the system of Mathisson—Papapetrou equations. For this purpose, in the first equation of this system we have to add a Lorentz force, which describes in first approximation the interaction of the nucleus with the quantum state averaging electromagnetic field of its electrons. Here, we neglect the terms, which contain the second derivative of 4-velocity and describe interaction between the nuclear magnetic moment and the field of electrons [14], because the numerical estimations show, that these terms are smaller than all other terms of the equation. In result we receive the following system of the equations:

$$\mu \frac{Du^i}{D\tau} = \frac{1}{2c} R^i{}_{jkl} u^j \varepsilon^{klpq} \bar{S}_p u_q + \frac{Ze}{c} F^{ij} u_j, \quad (2)$$

$$a) \frac{D\bar{S}^i}{D\tau} = \frac{1}{c^2} u^i \bar{S}_n \frac{Du^n}{D\tau}, \quad b) u^n \bar{S}_n = 0, \quad (3)$$

where Ze , $u^i = \frac{dx^i}{d\tau}$ and \bar{S}_n denote the charge, the 4-velocity and the classical spin of the nucleus respectively, here under the classical spin we understand the expectation value of the nuclear spin operator; ε^{klpq} is the Levi-Civita pseudotensor with $\varepsilon^{1234} = (-\det g_{ij})^{-1/2}$; $R^i{}_{jkl}$ is the Riemann curvature tensor; $F^i{}_j$ is the tensor of the electromagnetic field of electrons; c is the velocity of light. Here and everywhere the latin indexes run from 1 to 4, and greek ones from 1 to 3. The signature of the space-time metric is +2. We shall notice, that equation (3b) represents the additional Pirani condition [15]². Due to this condition it is possible to enter a 4-vector of a spin \bar{S}_k and constant μ , which we shall identify hereinafter with nuclear mass.

In the equation (2) of nuclear motion it is unknown only one quantity – the tensor of the average electromagnetic field F^{ij} , created by nuclear electrons. Thus, the problem about finding of the equations of motion of atom in an external gravitational field is reduced to calculation of the electromagnetic field of nuclear electrons. The most simple this problem can be decided in the special, comoving atom reference frame.

2 The Reference Frame of the Single Observer.

As a comoving reference frame we shall choose a reference frame of the single observer [17]. From our point of view, this reference frame is the most convenient for the description of objects of the small sizes.

The reference frame of the single observer is defined by a motion of a single mass point (“the single observer”). The world line of this mass point is named basis line. Along this line we establish a comoving tirade $h^i_{(k)}(\tau)$, determined by the condition $h^i_{(4)} = \frac{1}{c} u^i$ accurate to three-dimensional rotations. If we will use the world line of the nucleus (1) as a basis line, we will obtain a comoving reference frame for the atom.

²By force of assumptions made above, the Pirani condition coincides with the Tulczyjew-Dixon condition [14,16].

Three-dimensional physical space in the reference frame of the single observer we shall define as a geodesic spacelike hypersurface f , which is orthogonal to the basis line in the given moment of proper time τ . At each point P, laying on a hypersurface $P \in f(\tau)$, we shall put in conformity three scalars $X^{(\alpha)} = \sigma_P h_i^{(\alpha)} k^i$, which will hereinafter play a role of the three-dimensional coordinates. Here σ_P is the value of the conical parameter σ at the point P, defined along a spacelike geodesic in f ; k^i is the tangent unit vector to that geodesic at the point $\sigma = 0$.

For nonrotating frame (i.e. when the tirade $h_{(k)}^i(\tau)$ is set along a basic line with the help of Fermi—Walker transport) the quantities $(X^{(\alpha)}, c\tau)$ correspond to the Fermi normal coordinates, defined by Synge [17, 18]. In general case of rotating reference frame, the coordinates defined in the same way

$$x^{\bar{\alpha}} = X^{(\alpha)}, \quad x^{\bar{4}} = c\tau, \quad (4)$$

we shall name as rotating Fermi coordinates [19]. In these coordinates the metric tensor can be presented as:

$$g_{\bar{i}\bar{j}} = \eta_{(i)(j)} + \varepsilon_{(i)(j)}, \quad (5)$$

where

$$\varepsilon_{(\alpha)(\beta)} = -\frac{1}{3}R_{(\alpha)(\mu)(\beta)(\nu)}X^{(\mu)}X^{(\nu)} + O(\rho^3), \quad (6)$$

$$\varepsilon_{(\alpha)(4)} = \frac{1}{c}e_{(\alpha)(\sigma)(\tau)}X^{(\tau)}\omega^{(\sigma)} + \theta_{(\alpha)}, \quad (7)$$

$$\varepsilon_{(4)(4)} = -2\left(\frac{1}{c^2}W_{(\alpha)}X^{(\alpha)} + \theta\right), \quad (8)$$

$$\theta_{(\alpha)} = \frac{2}{3}R_{(\alpha)(\mu)(\nu)(4)}X^{(\mu)}X^{(\nu)} + O(\rho^3), \quad (9)$$

$$\theta = \frac{1}{2}\left(R_{(4)(\mu)(4)(\nu)} - \frac{1}{2}R_{(4)(\mu)(4)(\nu)(\tau)}X^{(\tau)}\right)X^{(\mu)}X^{(\nu)} + O(\rho^4). \quad (10)$$

Here, we used the following notations: $\eta_{(i)(j)} = \text{diag}(1, 1, 1, -1)$ is the Minkowski tensor;

$$W^{(\alpha)} = h_i^{(\alpha)} \frac{Du^i}{D\tau} \quad (11)$$

and

$$\omega^{(\alpha)} = \frac{1}{2}e^{(\alpha)(\kappa)(\tau)}h_{(\tau)i} \frac{Dh_{(\kappa)}^i}{D\tau} \quad (12)$$

are the acceleration and the angular velocity of the reference frame respectively; $e^{(\alpha)(\kappa)(\tau)}$ is the three-dimensional Levi-Civita symbol; $R^{(i)}_{(m)(n)(k)}$ and

$$R^{(i)}_{(m)(n)(k)(l)} = h_a^{(i)}h_{(m)}^b h_{(n)}^c h_{(k)}^d h_{(l)}^p R^a_{bcd;p} \quad (13)$$

are the tirade components of the Riemann curvature tensor and its covariant derivative respectively, determined along the basic line; $\rho = \sqrt{X_{(\alpha)}X^{(\alpha)}}$.

Because of the small sizes of atom, the condition $\varepsilon_{(i)(j)} \ll 1$ is allowable even for very strong (from the macroscopic point of view) gravitational fields, therefore for further calculations we shall be limited by consideration only linear terms in the $\varepsilon_{(i)(j)}$.

Taking into account that $u^{\bar{i}} = (0, 0, 0, c)$ and $g_{\bar{i}\bar{j}}(0) = \eta_{(i)(j)}$, we receive the following expressions for the system of Mathisson—Papapetrou equations in the rotating Fermi coordinates (4):

$$\mu W_{(\alpha)} = -ce^{(\mu)(\nu)(\tau)} R_{(4)(\nu)(\alpha)(\mu)} \bar{S}_{(\tau)} + ZeF_{(\alpha)(4)}, \quad (14)$$

$$\frac{d}{d\tau} \bar{S}_{(\alpha)} = e_{(\alpha)(\kappa)(\tau)} \omega^{(\tau)} \bar{S}^{(\kappa)}, \quad \bar{S}_{(4)} = 0, \quad (15)$$

where all quantities are taken along the nucleus world line ($X^{(\alpha)} = 0$).

3 Calculation of Electromagnetic Field of Electrons Inside the Atom.

To find how the electromagnetic field of electrons influences on the atom motion, it is necessary, first, solve the Maxwell equations in the Fermi coordinates for the electromagnetic field, created by electrons in the arbitrary point $\zeta^{(\alpha)}$. Second, calculate the expectation value of that field, using the assumption, that the atom is in a quasistationary quantum state.

Solving Maxwell equations

$$\left[\sqrt{-\det(g_{ij})} g^{mk} g^{nl} (A_{l,k} - A_{k,l}) \right]_{,n} = 0, \quad (16)$$

where $A_k = (A_{(\alpha)}, A_4 = -\varphi)$ is the electromagnetic potentials, we will interest only quasistationary solutions, i.e. we shall search the field of charges e , resting in the points $X_A^{(\alpha)}$ ($A = 1, 2, \dots, Z$). Avoiding in this case the consideration of the motion of electrons we neglect the effects of interaction of the magnetic field of electrons with the nucleus magnetic momentum. These effects are small enough because of the small velocity of electrons within the atom ($v \ll c$).

Writing down the Maxwell equations in the linear approximation in the $\varepsilon_{(i)(j)}$ and neglecting the terms, containing the derivative on time of the potentials, we will have the following expression for electromagnetic potentials of the system of the rest charges in some arbitrary point $\zeta^{(\alpha)}$:

$$\begin{aligned} \varphi(\zeta^{(\alpha)}) = \sum_{A=1}^Z \frac{e}{R_A} \left[1 + \frac{1}{2c^2} W_{(\beta)} R_A^{(\beta)} + \frac{1}{6} R_{(4)(\mu)(4)(\nu)} \zeta^{(\mu)} (2\zeta^{(\nu)} - X^{(\nu)}) + \right. \\ \left. + \frac{1}{6R_A^2} R_{(\beta)(\tau)(\nu)(\mu)} \zeta^{(\beta)} \zeta^{(\nu)} X_A^{(\tau)} X_A^{(\mu)} + O(\rho_A^3) \right], \end{aligned} \quad (17)$$

$$\begin{aligned} A^{(\sigma)}(\zeta^{(\alpha)}) = \sum_{A=1}^Z \frac{e}{R_A} \left[-\frac{1}{c} e^{(\sigma)}_{(\tau)(\nu)} X^{(\tau)} \omega^{(\nu)} - \frac{1}{6} R^{(\sigma)}_{(\nu)(4)(\tau)} \zeta^{(\nu)} \zeta^{(\tau)} + \right. \\ \left. + \frac{1}{2} R^{(\sigma)}_{(4)(\nu)(\tau)} \zeta^{(\nu)} X^{(\tau)} + \frac{1}{2} R^{(\sigma)}_{(\tau)(\nu)(4)} X^{(\nu)} X^{(\tau)} + O(\rho_A^3) \right], \end{aligned} \quad (18)$$

where $R_A^{(\alpha)} = (\zeta^{(\alpha)} - X_A^{(\alpha)})$, $R_A = \sqrt{R_A^{(\alpha)} R_{A(\alpha)}}$, $\rho_A = \sqrt{X_{A(\alpha)} X_A^{(\alpha)}}$.

Thus, we also assume, that inside of our system there is no substance or other strong fields, resulting to the additional curvature of space time, i.e. the Ricci tensor

inside of atom is equal to zero ($R_{ij} = 0$). Otherwise, the presence of the additional interaction would generate the effects, which exceed in magnitude the influence of the gravitational field on the atom motion.

Then, in comoving rotating Fermi coordinates the components of the tensor of the average electromagnetic field will be equal to:

$$F_{(\alpha)(4)} = \langle \hat{F}_{(\alpha)(4)} \rangle, \quad (19)$$

where

$$\begin{aligned} \hat{F}_{(\alpha)(4)} &\equiv - \left(\frac{\partial \hat{\varphi}(\zeta^{(\kappa)})}{\partial \zeta^{(\alpha)}} \right)_{\zeta^{(\nu)}=0} - \frac{1}{c} \left(\frac{\partial \hat{A}_{(\alpha)}}{\partial \tau} \right)_{\zeta^{(\nu)}=0} \approx \\ &\approx - \sum_{A=1}^Z \left(\frac{e \hat{X}_{A(\alpha)}}{\hat{\rho}_A^3} + \frac{e}{\hat{\rho}_A} \left(\frac{1}{3} R_{(\alpha)(4)(4)(\nu)} \hat{X}_A^{(\nu)} + \frac{1}{2c^2} W_{(\alpha)} \right) \right). \end{aligned} \quad (20)$$

Here, $\hat{X}_{A(\alpha)}$ is the position operator of A -th electron; $\hat{\rho}_A \equiv \sqrt{\hat{X}_{A(\alpha)} \hat{X}_A^{(\alpha)}}$ and the operators $\hat{\varphi}$ and \hat{A} are obtained from (17) and (18) by changing $X_A^{(\alpha)} \rightarrow \hat{X}_A^{(\alpha)}$, $\rho_A \rightarrow \hat{\rho}_A$ and so on.

In order to determine the expectation value (19) of the electromagnetic field tensor we will use the quasirelativistic two-component representation of the covariant Dirac equation. The detailed explanation of this representation, and the consistent formulation of the quantum mechanics in the arbitrary reference frames and in the external gravitational fields can be found in the book [8].

According to this approach [8], the covariant Dirac equation can be interpreted in general case as a special coordinate representation of the traditional quantum-mechanical equation of motion in Hilbert space. Thus, the problem about solving of the Dirac equation in the curved space-time can be lead to the similar problem of the traditional quantum mechanics in the flat space - time, and the properties of the reference frame and the curved space-time can be taken into account in the Hamiltonian as the additional potentials.

In particular, in quasirelativistic approximation our system can be described by a two-component Pauli-type equation

$$i\hbar \frac{\partial \psi}{\partial \tau} = \hat{H} \psi \quad (21)$$

(with

$$\int_f \psi^\dagger \psi d^3 X = 1, \quad (22)$$

and $d^3 X = dX^{(1)} dX^{(2)} dX^{(3)}$) in the reference frame of single observer. The complete expression for the two-component Hamiltonian \hat{H} (for one-electron atom) can be found in [8]. The analysis of the complete operator \hat{H} shows, that the influence of external gravitational field will always be more significant than effects caused by the non-Coulomb terms of the nuclear potentials³.

Therefore, in a good approximation the Hamiltonian of the system of Z electrons is given by:

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (23)$$

³The electromagnetic potentials of the nucleus can be obtained from (17) and (18) by the following substitution: $e \rightarrow Ze$, $\zeta_A^\alpha \leftrightarrow X_A^{(\alpha)}$, and $\zeta_A^\alpha \rightarrow 0$.

where

$$\hat{H}_0 = \sum_A \left(\frac{\hat{P}_A^2}{2m} - \frac{Ze^2}{\hat{\rho}_A} \right) + \frac{1}{2} \sum_{A \neq B} \frac{e^2}{\hat{\rho}_{AB}} \quad (24)$$

is the Hamiltonian of the multielectron atom in the flat space-time;

$$\begin{aligned} \hat{H}_1 = \sum_A \left[mc^2 \hat{\theta}_A + \frac{c}{2} \left(e^{(\sigma)(\alpha)(\tau)} \hat{\theta}_{A(\sigma),(\alpha)} \hat{S}_{A(\tau)} - \left\{ \hat{\theta}_A^{(\beta)}, \hat{P}_{A(\beta)} \right\} \right) - \right. \\ \left. - \omega^{(\beta)} \left(\hat{L}_{A(\beta)} + \hat{S}_{A(\beta)} \right) + mW_{(\beta)} \hat{X}_A^{(\beta)} \right] \end{aligned} \quad (25)$$

is the Hamiltonian, describing the interaction of the electrons with the external gravitational field. Here we introduced the following notations: $\hat{X}_A^{(\beta)} = X_A^{(\beta)}$, $\hat{P}_{A(\alpha)} = \frac{\hbar}{i} \partial / \partial \hat{X}_A^{(\alpha)}$, $\hat{L}_{A(\alpha)} = e_{(\alpha)(\beta)(\tau)} \hat{X}_A^{(\beta)} \hat{P}_A^{(\tau)}$ and $\hat{S}_{A(\alpha)} = \frac{\hbar}{2} \sigma_{(\alpha)}$ are the operators of the position, momentum, angular momentum and spin for the A -th electron; $A = 1, 2, \dots, Z$; $\sigma_{(\alpha)}$ are the standard Pauli matrices; $\hat{\theta}_{A(\alpha)} = \frac{2}{3} R_{(\alpha)(\mu)(\nu)(4)} \hat{X}_A^{(\mu)} \hat{X}_A^{(\nu)}$; $\hat{\rho}_{AB} = \sqrt{(\hat{X}_{A(\alpha)} - \hat{X}_{B(\alpha)})(\hat{X}_A^{(\alpha)} - \hat{X}_B^{(\alpha)})}$.

From (20) by using the symmetry of the non-disturbed stationary state of the atom, we have

$$\left\langle \hat{F}_{(\alpha)(4)} \right\rangle_0 = -\frac{e}{2c^2} W_{(\alpha)} \left\langle \sum_A \frac{1}{\hat{\rho}_A} \right\rangle_0, \quad (26)$$

where notation $\langle \dots \rangle_0$ means that the expectations values are calculated using eigenvectors of non-disturbed Hamiltonian \hat{H}_0 (24). If one neglects “deformation” of the atom by external gravitational field, then the electromagnetic field $F_{(\alpha)(4)}$ (see (19), (14)) will affect only renormalization of the nucleus mass $\mu \rightarrow \mu + \Delta\mu$, where $\Delta\mu = \frac{Ze^2}{2c^2} \left\langle \sum_A \frac{1}{\hat{\rho}_A} \right\rangle_0$. Because of $\Delta\mu/\mu \ll 1$, we will not hereinafter consider this renormalization.

Using perturbation theory, it is easy to show, that the required expectation value of the electromagnetic field tensor from equation (20) can be presented as [9]:

$$F_{(\alpha)(4)} = \left\langle \hat{F}_{(\alpha)(4)} \right\rangle = \left\langle \sum_A \left(-\frac{e\hat{X}_{A(\alpha)}}{\hat{\rho}_A^3} \right) \right\rangle + O(\varepsilon_{(\alpha)(\beta)}^2), \quad (27)$$

where $O(\varepsilon_{(\alpha)(\beta)}^2)$ denote the terms quadratic in $\varepsilon_{(i)(j)}$.

Direct calculation of quantity $\left\langle \sum_A \left(-\frac{e\hat{X}_{A(\alpha)}}{\hat{\rho}_A^3} \right) \right\rangle$ is connected with mathematical difficulties in the framework of the perturbation theory. Therefore we shall use the following property of the hermitian operators.

If observable L is described by the hermitian operator \hat{L} , which does not depend on time explicitly, the expectation value of the operator of evolution $\langle \hat{L} \rangle$ of this observable L in the stationary state (for which the state vector is an eigenvector of the Hamiltonian) will be equal to zero:

$$\frac{d}{dt} \langle \hat{L} \rangle = \langle \dot{\hat{L}} \rangle = 0, \quad (28)$$

where

$$\overset{\circ}{L} \equiv \left(\frac{\partial \hat{L}}{\partial \tau} \right)_{\text{expl}} + \frac{i}{\hbar} [\hat{H}, \hat{L}]. \quad (29)$$

In general case the Hamilton operator of the atom in an external gravitational field always explicitly depends on proper time τ . But, we can decompose the Hamiltonian H of our quantum system in a vicinity of an arbitrary moment of time τ_0 :

$$H(\tau) = H(\tau_0) + \left(\frac{\partial H}{\partial \tau} \right)_{\tau=\tau_0} (\tau - \tau_0) + \dots$$

and calculate the probabilities of transitions, caused by the term $\left(\frac{\partial H}{\partial \tau} \right)_{\tau=\tau_0} (\tau - \tau_0)$ in the operator H . If we will find, that during the time $(\tau - \tau_0) \sim \Delta\tau$ (where $\Delta\tau$ is the characteristic atomic time) these probabilities are much less than 1, we will consider the eigenvector of the operator H as the quasistationary state of the atom. Numerical estimations show, that this quasistationary conditions for atom states are satisfied for a wide class of gravitational fields (such as the external gravitational field of the macroscopic black holes). In our case, the terms included in the Hamiltonian \hat{H}_1 , such as $\hat{\theta}$ and $\hat{\theta}_{(\alpha)}$, are very slowly change with time. Therefore, even in case of the ultrarelativistic motion of the atom, when the atom passes a short distances during a characteristic atomic time, the gravitational field can be consider as homogeneous with a high precision (except of the case of short-wave gravitational radiation).

We can introduce the operators of 3-velocity $\overset{\circ}{X}_{A(\alpha)}$:

$$\begin{aligned} \overset{\circ}{X}_{A(\alpha)} &\equiv \left(\frac{\partial \hat{X}_{A(\alpha)}}{\partial \tau} \right)_{\text{expl}} + \frac{i}{\hbar} [\hat{H}, \hat{X}_{A(\alpha)}] \simeq \\ &\simeq \frac{1}{m} \hat{P}_{A(\alpha)} - \frac{2}{3} c R_{(\alpha)(\mu)(\nu)(4)} \hat{X}_A^{(\mu)} \hat{X}_A^{(\nu)} - e_{(\alpha)(\beta)(\tau)} \omega^{(\beta)} \hat{X}_A^{(\tau)}, \end{aligned} \quad (30)$$

and 3-acceleration $\overset{\circ\circ}{X}_{A(\alpha)}$:

$$\begin{aligned} \overset{\circ\circ}{X}_{A(\alpha)} &\equiv \left(\frac{\partial \overset{\circ}{X}_{A(\alpha)}}{\partial \tau} \right)_{\text{expl}} + \frac{i}{\hbar} [\hat{H}, \overset{\circ}{X}_{A(\alpha)}] \simeq \\ &\simeq \frac{1}{m} \left(\frac{Z e^2 \hat{X}_{A(\alpha)}}{\hat{\rho}_A^3} \right) + \frac{1}{m} \sum_{B, B \neq A} \left(\frac{e^2 (\hat{X}_{A(\alpha)} - \hat{X}_{B(\alpha)})}{2 \hat{\rho}_{AB}^3} \right) - c^2 \hat{\theta}_{A,(\alpha)} - \\ &\quad - \frac{c}{2m} e^{(\sigma)(\beta)(\tau)} \hat{\theta}_{A(\sigma),(\beta),(\alpha)} \hat{S}_{A(\tau)} - \frac{ci}{2m\hbar} [\{\hat{\theta}_A^{(\beta)}, \hat{P}_{A(\beta)}\}, \hat{P}_{A(\alpha)}] + \\ &\quad + \frac{1}{m} \omega^{(\beta)} e_{(\beta)(\alpha)(\tau)} \hat{P}_A^{(\tau)} - W_{(\alpha)} \end{aligned} \quad (31)$$

By direct calculation it is possible to show, that, if the atom is in a quasistationary state, the operators of 3-velocity $\overset{\circ}{X}_{A(\alpha)}$ and 3-acceleration $\overset{\circ\circ}{X}_{A(\alpha)}$ for each electron satisfy to the following equations:

$$\langle \overset{\circ}{X}_{A(\alpha)} \rangle = 0, \quad \langle \overset{\circ\circ}{X}_{A(\alpha)} \rangle = 0. \quad (32)$$

Taking into account the obvious explicit time-independence of the operators $\hat{X}_A^{(\alpha)}$ and $\hat{P}_A^{(\alpha)}$ and the fact, that they satisfy to following commutation relations:

$$[\hat{P}_A^{(\alpha)}, \hat{X}_B^{(\beta)}] = \frac{\hbar}{i} \delta^{(\alpha)(\beta)} \delta_{AB}, \quad (33)$$

$$[\hat{X}_A^{(\alpha)}, \hat{X}_B^{(\beta)}] = 0, \quad [\hat{P}_A^{(\alpha)}, \hat{P}_B^{(\beta)}] = 0, \quad (34)$$

we receive from system of the equations (32) the following expression:

$$\begin{aligned} & \left\langle \sum_A \left(-\frac{Ze^2 \hat{X}_{A(\alpha)}}{\hat{\rho}_A^3} \right) \right\rangle \cong -ZmW^{(\alpha)} - \\ & - \left\langle \sum_A \left[mc^2 \hat{\theta}_{A,(\alpha)} - ce^{(\sigma)(\delta)(\tau)} R_{(\alpha)(\delta)(4)(\sigma)} \left(\hat{S}_{A(\tau)} + \hat{L}_{A(\tau)} \right) \right] \right\rangle, \end{aligned} \quad (35)$$

where we used, that “gravitational potentials” $\hat{\theta}$ and $\hat{\theta}_{(\alpha)}$ very slowly vary with time:

$$m \left\langle \hat{\theta}_{(\kappa)} \right\rangle \cong R_{(4)(\mu)(\kappa)(\nu)} \left\langle \left\{ \hat{X}^{(\mu)}, \hat{P}^{(\nu)} \right\} \right\rangle \cong 0. \quad (36)$$

Because of we neglect of quadratic terms in $\varepsilon_{(i)(j)}$, we can change from $\langle \dots \rangle$ to $\langle \dots \rangle_0$, where notation $\langle \dots \rangle_0$ means that the expectation value is calculated in relation to eigenvectors of non-disturbed operator (24). Then we receive from the system (14) (15) the following expression for the equation of motion of the multielectron atom in an external gravitational field in the comoving reference frame:

$$\begin{aligned} & (\mu + Zm) W_{(\alpha)} = -ce^{(\sigma)(\nu)(\tau)} R_{(4)(\nu)(\alpha)(\sigma)} \left[\bar{S}_{(\tau)} + \right. \\ & \left. + \left\langle \sum_A \left(\hat{S}_{A(\tau)} + \hat{L}_{A(\tau)} \right) \right\rangle \right] - mc^2 \left\langle \sum_A \hat{\theta}_{A,(\alpha)} \right\rangle_0. \end{aligned} \quad (37)$$

The second term in the right part of the received equation (37)

$$\begin{aligned} & -mc^2 \left\langle \sum_A \hat{\theta}_{A,(\alpha)} \right\rangle_0 = \frac{1}{4} mc^2 \left[R_{(4)(\mu)(4)(\alpha)(\tau)} + \right. \\ & \left. + R_{(4)(\tau)(4)(\mu)(\alpha)} + R_{(4)(\alpha)(4)(\tau)(\mu)} \right] \left\langle \sum_A \hat{X}_A^{(\mu)} \hat{X}_A^{(\tau)} \right\rangle_0 \end{aligned} \quad (38)$$

describes the interaction of an external gravitational field with the average quadrupole moment of atom. From estimations made above, this term becomes actually small for atomic dimensions, if we assume, that the full spin of the atom (which consists of the spins of the nucleus and electrons, and also of the electronic orbital moment) is not equal to zero. The calculations of the expectation values of the operator $\sum_A \left(\hat{L}_{A(\alpha)} + \hat{S}_{A(\alpha)} \right)$ describing variation of the electron angular momentum, by means of (3) lead us to

$$\frac{d}{d\tau} \left[\bar{S}_{(\alpha)} + \left\langle \sum_A (\hat{L}_{A(\alpha)} + \hat{S}_{A(\alpha)}) \right\rangle \right] \cong$$

$$\cong e_{(\alpha)}^{(\nu)(\kappa)} \omega_{(\kappa)} \left[\bar{S}_{(\nu)} + \left\langle \sum_A (\hat{L}_{A(\nu)} + \hat{S}_{A(\nu)}) \right\rangle_0 \right]. \quad (39)$$

Finally, the equation of motion of the multielectron atom it is possible to write down as:

$$(\mu + Zm) W_{(\alpha)} = -ce^{(\sigma)(\nu)(\tau)} R_{(4)(\nu)(\alpha)(\sigma)} \left[\bar{S}_{(\tau)} + \left\langle \sum_A (\hat{S}_{A(\tau)} + \hat{L}_{A(\tau)}) \right\rangle_0 \right]. \quad (40)$$

In this way, we have demonstrated, using the some physically reasonable assumptions, that the motion of multielectron atom in an external gravitational field in a good approximation can be described by the system of classical Mathisson—Papapetrou equations

$$(\mu + Zm) \frac{Du^i}{D\tau} = \frac{1}{2c} R^i_{jkl} u^j \varepsilon^{klmn} u_n J_m, \quad (41)$$

$$\frac{DJ^i}{D\tau} = \frac{1}{c^2} u^i J_n \frac{Du^i}{D\tau}, \quad J_m u^m = 0, \quad (42)$$

if we put as a classical angular momentum of atom the expectation value of the operator J^k of the total angular momentum of the system. In comoving rotating Fermi coordinates the quantity J^k has the following components:

$$J_{(\alpha)} = \bar{S}_{(\alpha)} + \left\langle \sum_A (\hat{L}_{A(\alpha)} + \hat{S}_{A(\alpha)}) \right\rangle_0, \quad J_{(4)} = 0. \quad (43)$$

We note that if we also consider the influence of any external electromagnetic field ${}^{(0)}F^{ij}$ on the atom motion, we have to add in the equation (41) the following terms:

$$\frac{e}{c} (Z + 1) {}^{(0)}F^{ij} u_j + \frac{1}{c} {}^{(0)}F^i_{m;n} \varepsilon^{mnkl} M_k u_l, \quad (44)$$

where M_k is the 4-vector of the atoms full magnetic moment, which in comoving reference frame has the the following components:

$$M_{(\alpha)} = \frac{e}{2mc} \left\langle \sum_A (\hat{\mathcal{L}}_{(\alpha)} + 2\hat{S}_{(\alpha)}) \right\rangle_0 + \frac{Zeg}{2\mu c} \bar{S}_{(\alpha)}, \quad M_{(4)} = 0. \quad (45)$$

As it is visible from the received equation (40), the trajectory of the atom will depend on the total angular momentum of the atom, which includes spins of the nucleus and electrons, and also orbital moment of electrons in atom. Hence, the motion of the atom in many respects depends on his quantum state. So, for example, the atoms, being in states with different mutual orientations of spins of the nuclear electrons, will move in general case along the different trajectories in an external gravitational field. Besides, the atoms, being in excited states with long life time, will be separated by an external gravitational field from atoms, which being in nonexcited states. Thus, the ultrarelativistic motion of atoms in the external gravitational fields can lead to a set of generally-relativistic effects, which can represent interest for astrophysics and allow us to check up the predictions of the general relativity on the quantum level.

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